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(6) OPTICAL AND MAGNETIC RESONANCE STUDIES OF ENERGY TRANSFER IN INORGANIC MOLECULAR SOLIDS

(9) FINAL REPORT, 1 Jan 77 — 31 May 80

by

(10) Elliot R. Bernstein
Principal Investigator

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The view, opinions, and/or findings contained in this report are those of the author and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

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vibronic coupling
electron paramagnetic resonance
energy transfer
Raman scattering

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report summarizes the important results of the grant research. It includes a statement of the problem studied, a list of personnel supported during the life of the grant, and a list of publications which resulted from the supported research.

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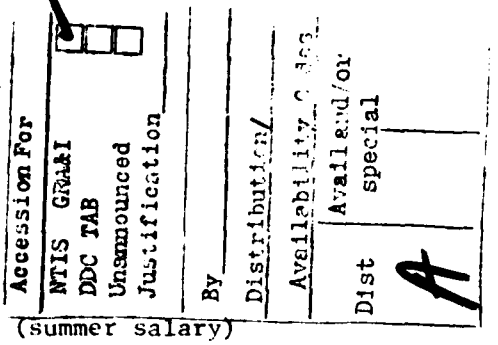
Statement of Problem Studied

Optical and magnetic resonance investigations of inorganic molecular solids were performed. We have studied magnetic resonance, Raman scattering, and optical spectra of various transition metal hexafluorides. The aim of these studies was to begin a program to determine the dynamical energy properties of transition metal molecular crystal systems.



Scientific Personnel Supported During This Period

Lawrence Dennis, Postdoctoral Fellow

Daniel Michalopoulos, Graduate Student

John D. Webb, Graduate Student

Elliot R. Bernstein, Principal Investigator (summer salary)

Summary of Important Results

The important results for this research fall into two categories. The first is a study of the Jahn Teller Effect in iridium hexafluoride (IrF_6). This work is significant because it lays the foundation for a detailed analysis of the vibronic coupling in molecules and solids. The careful analysis of three of the degenerate electronic states of IrF_6 by absorption and Raman scattering studies of low temperature crystals has enabled us to determine linear and quadratic vibronic coupling parameters and how vibronic coupling interferes with interactions in the solid. We have performed a theoretical analysis of the energy levels of IrF_6.

The second area of important contributions is in the analysis of electron paramagnetic resonance data for an octahedral Γ_8 state. We have demonstrated for the first time that such a state, even in a cubic environment, evidences anisotropic behavior and highly complicated magnetic resonanace spectra.

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